Reference

NBS
PUBLICATIONS

A11102 491786

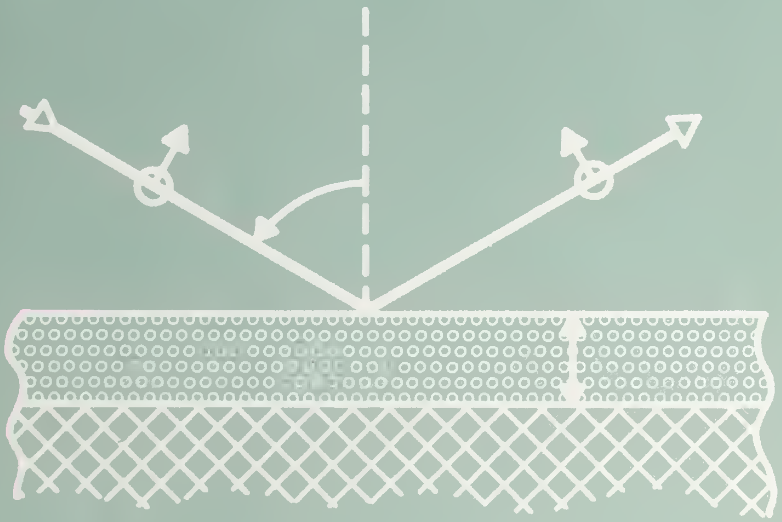
NAT'L INST OF STANDARDS & TECH R.I.C.
A11102491786
Chandler-Horowitz, D/Analytic analysis o
QC100 .U57 NO.400-78 V1986 C.1 NBS-PUB-R

NBS SPECIAL PUBLICATION **400-78**

U.S. DEPARTMENT OF COMMERCE/National Bureau of Standards

Semiconductor Measurement Technology:

Analytic Analysis of Ellipsometric Errors



$$\begin{matrix}\psi \pm \delta\psi,\ \Delta \pm \delta\Delta \\ \phi \pm \delta\phi,\ n_s \pm \delta n_s\end{matrix} \longrightarrow \text{EEA} \longrightarrow \begin{matrix} t \pm \delta t \\ n_f \pm \delta n_f\end{matrix}$$

Deane Chandler-Horowitz

QC
100
.U57
#400-78
1986

The National Bureau of Standards[1] was established by an act of Congress on March 3, 1901. The Bureau's overall goal is to strengthen and advance the nation's science and technology and facilitate their effective application for public benefit. To this end, the Bureau conducts research and provides: (1) a basis for the nation's physical measurement system, (2) scientific and technological services for industry and government, (3) a technical basis for equity in trade, and (4) technical services to promote public safety. The Bureau's technical work is performed by the National Measurement Laboratory, the National Engineering Laboratory, the Institute for Computer Sciences and Technology, and the Institute for Materials Science and Engineering.

The National Measurement Laboratory

Provides the national system of physical and chemical measurement; coordinates the system with measurement systems of other nations and furnishes essential services leading to accurate and uniform physical and chemical measurement throughout the Nation's scientific community, industry, and commerce; provides advisory and research services to other Government agencies; conducts physical and chemical research; develops, produces, and distributes Standard Reference Materials; and provides calibration services. The Laboratory consists of the following centers:

- Basic Standards[2]
- Radiation Research
- Chemical Physics
- Analytical Chemistry

The National Engineering Laboratory

Provides technology and technical services to the public and private sectors to address national needs and to solve national problems; conducts research in engineering and applied science in support of these efforts; builds and maintains competence in the necessary disciplines required to carry out this research and technical service; develops engineering data and measurement capabilities; provides engineering measurement traceability services; develops test methods and proposes engineering standards and code changes; develops and proposes new engineering practices; and develops and improves mechanisms to transfer results of its research to the ultimate user. The Laboratory consists of the following centers:

- Applied Mathematics
- Electronics and Electrical Engineering[2]
- Manufacturing Engineering
- Building Technology
- Fire Research
- Chemical Engineering[2]

The Institute for Computer Sciences and Technology

Conducts research and provides scientific and technical services to aid Federal agencies in the selection, acquisition, application, and use of computer technology to improve effectiveness and economy in Government operations in accordance with Public Law 89-306 (40 U.S.C. 759), relevant Executive Orders, and other directives; carries out this mission by managing the Federal Information Processing Standards Program, developing Federal ADP standards guidelines, and managing Federal participation in ADP voluntary standardization activities; provides scientific and technological advisory services and assistance to Federal agencies; and provides the technical foundation for computer-related policies of the Federal Government. The Institute consists of the following centers:

- Programming Science and Technology
- Computer Systems Engineering

The Institute for Materials Science and Engineering

Conducts research and provides measurements, data, standards, reference materials, quantitative understanding and other technical information fundamental to the processing, structure, properties and performance of materials; addresses the scientific basis for new advanced materials technologies; plans research around cross-country scientific themes such as nondestructive evaluation and phase diagram development; oversees Bureau-wide technical programs in nuclear reactor radiation research and nondestructive evaluation; and broadly disseminates generic technical information resulting from its programs. The Institute consists of the following Divisions:

- Ceramics
- Fracture and Deformation[3]
- Polymers
- Metallurgy
- Reactor Radiation

---

[1] Headquarters and Laboratories at Gaithersburg, MD, unless otherwise noted; mailing address Gaithersburg, MD 20899.

[2] Some divisions within the center are located at Boulder, CO 80303.

[3] Located at Boulder, CO, with some elements at Gaithersburg, MD.

NBS
RESEARCH
INFORMATION
CENTER

Semiconductor Measurement Technology:

Analytic Analysis of Ellipsometric Errors

Deane Chandler-Horowitz

Semiconductor Electronics Division
Center for Electronics and Electrical Engineering
National Engineering Laboratory
Gaithersburg, MD 20899

U.S. DEPARTMENT OF COMMERCE, Malcolm Baldrige, Secretary
NATIONAL BUREAU OF STANDARDS, Ernest Ambler, Director

Issued May 1986

Library of Congress Catalog Card Number: 86-600541

National Bureau of Standards Special Publication 400-78
Natl. Bur. Stand. (U.S.), Spec. Publ. 400-78, 36 pages (May 1986)
CODEN: XNBSAV

U.S. GOVERNMENT PRINTING OFFICE
WASHINGTON: 1986

For sale by the Superintendent of Documents, U.S. Government Printing Office, Washington, DC 20402

Table of Contents

Page

Abstract 1

Introduction 1

Theory and Calculations 2

Program Description 8

Example Program Outputs 10

Conclusions 10

Acknowledgments 11

References 11

Appendix 18

List of Figures

1. Program flow chart 12

2. Plot of percent error in thickness and error in refractive index for a silicon dioxide film 100 nm thick on a silicon substrate 13

3. Plot of percent error in thickness and error in refractive index for a silicon dioxide film 10 nm thick on a silicon substrate 14

4. Plot of percent error in thickness and error in refractive index for a silicon dioxide film 280 nm thick on a silicon substrate 15

5. Plot of percent error in thickness and error in refractive index for a silicon nitride film 80 nm thick on a silicon substrate 16

6. Plot of error in refractive index (real part) and error in refractive index (imag part) for a bare silicon substrate 17

Semiconductor Measurement Technology: Analytic Analysis of Ellipsometric Errors

Deane Chandler-Horowitz
Semiconductor Electronics Division
National Bureau of Standards
Gaithersburg, MD 20899

Abstract

A computer program is given that contains an explicit error analysis (EEA) for ellipsometric measurements. The program can identify the ellipsometric inaccuracies for any ellipsometer, can be used to determine which parameters contribute the most to the overall measurement inaccuracy, and can lead one to an optimum measurement procedure. A FORTRAN program that performs the evaluation of the partial derivative expressions needed to analyze ellipsometric measurement uncertainties is listed. The program determines the uncertainty in the calculation of the refractive index of a bare isotropic substrate or the uncertainty in the determination of the thickness and refractive index of a nonabsorbing film on a substrate of known refractive index. These are the two most commonly used surface models used in ellipsometry performed at single angle of incidence and a single wavelength. The program input parameters include the wavelength of light, the angle of incidence and its uncertainty, and the uncertainties in the ellipsometric parameters Δ and ψ. They also include in the ambient-substrate model an estimated value for the substrate's refractive index, and in the film-substrate model the refractive index of the substrate and its uncertainty and estimated values for the film's refractive index and thickness. The case of the conventional null ellipsometer utilizing a quarter-wave plate is treated to find the uncertainties in Δ and ψ from the uncertainties in the polarizer and analyzer null values and the waveplate constants.

Key words: bare substrate model; computer program; ellipsometric error analysis; film refractive index; film-substrate model; film thickness; substrate refractive index.

Introduction

A FORTRAN program was developed that calculates the ellipsometric measurement uncertainties for two models of a surface. The first is the simple bare isotropic substrate model. The second is the isotropic nonabsorbing film-substrate model. It is assumed that the sample to be measured ellipsometrically can be best described by one of these two models. From the ellipsometer, one obtains values for the two angular quantities Δ and ψ. These allow a determination of at least two of the unknown optical properties of the surface. This corresponds to a determination of the real and imaginary parts of the substrate refractive index for the bare substrate model and a determination of the film's refractive index and thickness for the film-substrate model. In each case, a calculation involving the inversion of the ellipsometric equations is performed to solve for the unknown optical properties [1].

For an ideal ellipsometer, Δ and ψ are functions of up to six independent parameters: the ambient refractive index, the substrate refractive index, the film refractive index and thickness, the angle of incidence, and the wavelength. The measured or assumed values of these parameters may have systematic errors in addition to random errors. In an actual ellipsometer, the measured values of Δ and ψ are susceptible to other sources of errors. These can include azimuthal-angle errors, component and cell-window optical imperfections, beam deviation errors, parasitic beams, source-beam polarization and collimation errors, polarization-dependent detector sensitivity, and residual mechanical imperfections. Therefore, the ultimate accuracy for a nonideal ellipsometer can be limited by these other errors, and, for a further error investigation, one should assess the above errors. In the case of the conventional null instrument, the method of measuring Δ and ψ using four-zone averaging best ensures that Δ and ψ are free from most above cited imperfections [2]. The analytic functions for Δ and ψ can then be solved for the two unknown differentials that lead to a calculation of the uncertainty in the ellipsometrically measured quantities[3,4].

Theory and Calculations

The ellipsometric parameters Δ and ψ are defined by the complex reflectance ratio ρ as follows [5]:

$$\rho = \frac{R_p}{R_s} = tan\psi \; e^{i\Delta}. \tag{1}$$

Here, R_p and R_s are the ratios of the reflected to the incident electric field amplitudes of the light for polarization parallel, p, and perpendicular, s, to the plane of incidence. In the case of light reflection from the ambient-substrate surface, the complex reflectances are:

$$R_p = \frac{n_s \; cos\phi - n_0\sqrt{1 - \left[\dfrac{n_0 \; sin\phi}{n_s}\right]^2}}{n_s \; cos\phi + n_0\sqrt{1 - \left[\dfrac{n_0 \; sin\phi}{n_s}\right]^2}} \tag{2}$$

$$R_s = \frac{n_0 \; cos\phi - n_s\sqrt{1 - \left[\dfrac{n_0 \; sin\phi}{n_s}\right]^2}}{n_0 \; cos\phi + n_s\sqrt{1 - \left[\dfrac{n_0 \; sin\phi}{n_s}\right]^2}}. \tag{3}$$

In the case of the ambient-film-substrate model, the reflectances are:

$$R_p = \frac{r_{p0f} + r_{pfs} \; e^{-i2\beta}}{1 + r_{p0f} \; r_{pfs} \; e^{-i2\beta}} \tag{4}$$

$$R_s = \frac{r_{s0f} + r_{sfs}\ e^{-i2\beta}}{1 + r_{s0f}\ r_{sfs}\ e^{-i2\beta}}, \tag{5}$$

where

$$r_{p0f} = \frac{n_f\ cos\phi - n_0\sqrt{1 - \left[\frac{n_0\ sin\phi}{n_f}\right]^2}}{n_f\ cos\phi + n_0\sqrt{1 - \left[\frac{n_0\ sin\phi}{n_f}\right]^2}} \tag{6}$$

$$r_{s0f} = \frac{n_0\ cos\phi - n_f\sqrt{1 - \left[\frac{n_0\ sin\phi}{n_f}\right]^2}}{n_0\ cos\phi + n_f\sqrt{1 - \left[\frac{n_0\ sin\phi}{n_f}\right]^2}} \tag{7}$$

$$r_{pfs} = \frac{n_s\sqrt{1 - \left[\frac{n_0\ sin\phi}{n_f}\right]^2} - n_f\sqrt{1 - \left[\frac{n_0\ sin\phi}{n_s}\right]^2}}{n_s\sqrt{1 + \left[\frac{n_0\ sin\phi}{n_f}\right]^2} + n_f\sqrt{1 - \left[\frac{n_0\ sin\phi}{n_s}\right]^2}} \tag{8}$$

$$r_{sfs} = \frac{n_f\sqrt{1 - \left[\frac{n_0\ sin\phi}{n_f}\right]^2} - n_s\sqrt{1 - \left[\frac{n_0\ sin\phi}{n_s}\right]^2}}{n_f\sqrt{1 + \left[\frac{n_0\ sin\phi}{n_f}\right]^2} + n_s\sqrt{1 - \left[\frac{n_0\ sin\phi}{n_s}\right]^2}}. \tag{9}$$

r_{p0f} and r_{s0f} are the real Fresnel reflection coefficients for the p and s polarizations of the electric field for the air-film interface. r_{pfs} and r_{sfs} are the corresponding complex Fresnel coefficients for the film-substrate interface. The refractive indices are n_0 for the ambient, n_f for the film, and n_s for the substrate. The angle of incidence is ϕ and the film phase thickness β is given in terms of the wavelength, λ, and film thickness, t, as follows:

$$\beta = \frac{2\ \pi\ t\ n_f}{\lambda}\sqrt{1 - \left[\frac{n_0\ sin\phi}{n_f}\right]^2}. \tag{10}$$

It should be noted that there is no explicit dependence on wavelength for the bare substrate model case.

The measurement uncertainties are derived for the bare substrate model as follows. The function ρ as given by eq (1) is a function of n_0, n_s, and ϕ:

$$\rho = \rho(n_0,\ n_s,\ \phi). \tag{11}$$

The substrate's refractive index has, in general, a real and imaginary part:

$$n_s = n_{sr} - i\ n_{si}. \tag{12}$$

n_{sr} is the real part of the index of refraction, and n_{si} is the imaginary part, normally expressed as the extinction coefficient k.

By taking the total differential of eq (11), $d\rho$, and assuming the differential quantities $d\Delta$, $d\psi$, dn_0, $d\phi$ correspond to experimentally known uncertainties, the following result for the uncertainty of n_s is obtained, neglecting the variation in n_0:

$$dn_s = \frac{d\rho - \dfrac{\partial \rho}{\partial \phi}\, d\phi}{\dfrac{\partial \rho}{\partial n_s}}. \tag{13}$$

By eq (1), this expands to

$$dn_s = \frac{i\ \rho\ d\Delta + sec^2\psi\ e^{i\Delta}\ d\psi - \dfrac{\partial \rho}{\partial \phi}\, d\phi}{\dfrac{\partial \rho}{\partial n_s}}. \tag{14}$$

From eqs (1), (2), and (3),

$$\frac{\partial \rho}{\partial n_s} = -\frac{n_s\ (1+\rho)^3\ cos^2\phi}{2\ (1-\rho)\ n_0{}^2\ sin^4\phi} \tag{15}$$

and

$$\frac{\partial \rho}{\partial \phi} = -\frac{\dfrac{\partial \rho}{\partial n_s}\ [n_s{}^2\ (1+sec^2\phi) + n_0{}^2(1-sec^2\phi)]}{n_s\ tan\phi}. \tag{16}$$

Therefore,

$$dn_s = a_1\ d\phi + a_2\ d\Delta + a_3\ d\psi, \tag{17}$$

where

$$a_1 = \frac{[n_s{}^2\ (1+sec^2\phi) + n_0{}^2\ (1-sec^2\phi)]}{n_s\ tan\phi} \tag{18}$$

$$a_2 = 2\ i\ \rho\ \frac{\rho - 1}{n_s\ (1+\rho)^3}\ n_0{}^2\ sin^2\phi\ tan^2\phi \tag{19}$$

$$a_3 = 2\ \frac{\rho - 1}{n_s\ (1+\rho)^3}\ n_0{}^2\ sin^2\phi\ tan^2\phi\ sec^2\psi\ e^{i\Delta} \tag{20}$$

and

$$dn_{sr} = real(dn_s) \quad and \quad dn_{si} = imag(dn_s). \tag{21}$$

Here, dn_{sr} and dn_{si} are the differentials in the substrate's real and imaginary parts of refractive index. This leads to a standard deviation of the ellipsometrically measured quantities n_{sr} and n_{si} as follows:

$$\sigma_{nsr} = \sqrt{real^2(a_1)\ \sigma_\phi^2 + real^2(a_2)\ \sigma_\Delta^2 + real^2(a_3)\ \sigma_{psi}^2} \tag{22}$$

$$\sigma_{nsi} = \sqrt{imag^2(a_1)\ \sigma_\phi^2 + imag^2(a_2)\ \sigma_\Delta^2 + imag^2(a_3)\ \sigma_{psi}^2}, \tag{23}$$

where σ_ϕ, σ_Δ, and σ_{psi} are the standard deviations of ϕ, Δ, and ψ when the measurement errors are random. This present FORTRAN program calculates the maximum uncertainty for treating systematic errors, which are more likely for an ellipsometer, and gives the uncertainties in n_{sr} and n_{si} as:

$$\delta n_{sr} = |real(a_1)\ \delta\psi| + |real(a_2)\ \delta\Delta| + |real(a_3)\ \delta\phi| \tag{24}$$

$$\delta n_{si} = |imag(a_1)\ \delta\psi| + |imag(a_2)\ \delta\Delta| + |imag(a_3)\ \delta\phi|, \tag{25}$$

where δ represents systematic measurement uncertainties.

The film-substrate uncertainty equations are more complicated but are derived as follows. Δ and ψ from eq (1) have the following functional form:

$$\Delta = \Delta(\phi,\ \lambda,\ n_0,\ n_f,\ t,\ n_s) \tag{26}$$

$$\psi = \psi(\phi,\ \lambda,\ n_0,\ n_f,\ t,\ n_s). \tag{27}$$

By taking the total differential of eqs (26) and (27) and then assuming all variations are known except the variations in film thickness, dt, and refractive index, dn_f, the following results of the solution for dt and dn_f are obtained, neglecting the variations in n_0 and λ:

$$dt = \frac{1}{k_1}\ [b_1\ d\psi + b_2\ d\Delta + b_3\ d\phi + b_4\ dn_{sr} + b_5\ dn_{si}] \tag{28}$$

$$dn_f = \frac{1}{k_1}\ [c_1\ d\psi + c_2\ d\Delta + c_3\ d\phi + c_4\ dn_{sr} + c_5\ dn_{si}], \tag{29}$$

where

$$b_1 = \frac{\partial\Delta}{\partial n_f} \tag{30}$$

$$b_2 = \frac{\partial\psi}{\partial n_f} \tag{31}$$

$$b_3 = \frac{\partial\Delta}{\partial\phi}\frac{\partial\psi}{\partial n_f} - \frac{\partial\psi}{\partial\phi}\frac{\partial\Delta}{\partial n_f} \tag{32}$$

$$b_4 = \frac{\partial\Delta}{\partial n_{sr}}\frac{\partial\psi}{\partial n_f} - \frac{\partial\psi}{\partial n_{sr}}\frac{\partial\Delta}{\partial n_f} \tag{33}$$

$$b_5 = \frac{\partial\Delta}{\partial n_{si}}\frac{\partial\psi}{\partial n_f} - \frac{\partial\psi}{\partial n_{si}}\frac{\partial\Delta}{\partial n_f} \tag{34}$$

$$c_1 = \frac{\partial\Delta}{\partial t} \tag{35}$$

$$c_2 = \frac{\partial\psi}{\partial t} \tag{36}$$

$$c_3 = \frac{\partial\Delta}{\partial\phi}\frac{\partial\psi}{\partial t} - \frac{\partial\psi}{\partial\phi}\frac{\partial\Delta}{\partial t} \tag{37}$$

$$c_4 = \frac{\partial\Delta}{\partial n_{sr}}\frac{\partial\psi}{\partial t} - \frac{\partial\psi}{\partial n_{sr}}\frac{\partial\Delta}{\partial t} \tag{38}$$

$$c_5 = \frac{\partial\Delta}{\partial n_{si}}\frac{\partial\psi}{\partial t} - \frac{\partial\psi}{\partial n_{si}}\frac{\partial\Delta}{\partial t} \tag{39}$$

and

$$k_1 = \frac{\partial\psi}{\partial n_f}\frac{\partial\Delta}{\partial t} - \frac{\partial\Delta}{\partial n_f}\frac{\partial\psi}{\partial t}. \tag{40}$$

The uncertainties for the two measured quantities t and n_f are then

$$\delta t = \frac{1}{|k_1|}\left[|b_1\ \delta\psi| + |b_2\ \delta\Delta| + |b_3\ \delta\phi| + |b_4\ \delta n_{sr}| + |b_5\ \delta n_{si}|\right] \tag{41}$$

$$\delta n_f = \frac{1}{|k_1|}\left[|c_1\ \delta\psi| + |c_2\ \delta\Delta| + |c_3\ \delta\phi| + |c_4\ \delta n_{sr}| + |c_5\ \delta n_{si}|\right]. \tag{42}$$

The desired partial derivatives contained in eqs (30) through (40) are derived explicitly from eq (1) by first taking the partial derivative of eq (1) with respect to either t, n_f, ϕ, n_{sr}, or n_{si}. For example, to find the quantities $\frac{\partial\psi}{\partial t}$ and $\frac{\partial\Delta}{\partial t}$, one gets[6]:

$$\left[sec^2\psi\ \frac{\partial\psi}{\partial t} + i\ tan\psi\ \frac{\partial\Delta}{\partial t}\right] e^{i\Delta} = \frac{\partial\left(\frac{R_p}{R_s}\right)}{\partial t} = tan\psi\ e^{i\Delta}\ C, \tag{43}$$

where C is defined as

$$C = \frac{1}{R_p}\frac{\partial R_p}{\partial t} - \frac{1}{R_s}\frac{\partial R_s}{\partial t}. \tag{44}$$

By separating eq (43) into its real and imaginary parts, one obtains for the solutions for $\frac{\partial\psi}{\partial t}$ and $\frac{\partial\Delta}{\partial t}$:

$$\frac{\partial\psi}{\partial t} = \frac{sin2\psi}{2}\ real(C) \tag{45}$$

and

$$\frac{\partial\Delta}{\partial t} = imag(C). \tag{46}$$

The following calculation allows one to determine the uncertainties in Δ and ψ when performing the conventional null ellipsometric measurement in one zone with an ideal ellipsometer having a simple quarter-wave plate. The uncertainties in the calculated values for Δ and ψ can be calculated from the uncertainties in the polarizer and analyzer null positions, P and A, and the quarter-wave plate's azimuth angle, Q, transmittance ratio, T_c, and relative phase retardation, Δ_c, uncertainties. From eq (1)

$$\Delta = tan^{-1}\left[\frac{imag(\rho)}{real(\rho)}\right] \tag{47}$$

and

$$\psi = tan^{-1}\sqrt{imag^2(\rho) + real^2(\rho)}. \tag{48}$$

For this ellipsometer [7],

$$\rho = \frac{tanA[tanQ + \rho_c \, tan(P-Q)]}{\rho_c \, tanQ \, tan(P-Q) - 1} = \rho_r + i \, \rho_i, \tag{49}$$

where ρ_c for the waveplate is given by

$$\rho_c = T_c \, e^{i\Delta_c}. \tag{50}$$

ρ_r and ρ_i are the real and imaginary parts of ρ. ρ_c is a complex number characterizing waveplate by the ratio, T_c, of the transmittance along its fast axis to the transmittance along its slow axis and the relative phase retardation, Δ_c, between these two axes.

The differentials of Δ and ψ are given by

$$d\Delta = \frac{1}{k_2} \, [d_1 \, dP + d_2 \, dA + d_3 \, dQ + d_4 \, dT_c + d_5 \, d\Delta_c] \tag{51}$$

and

$$d\psi = \frac{1}{k_3} \, [e_1 \, dP + e_2 \, dA + e_3 \, dQ + e_4 \, dT_c + e_5 \, d\Delta_c], \tag{52}$$

where

$$d_1 = \frac{\partial \rho_i}{\partial P} - \frac{\rho_i}{\rho_r}\frac{\partial \rho_r}{\partial P} \tag{53}$$

$$d_2 = \frac{\partial \rho_i}{\partial A} - \frac{\rho_i}{\rho_r}\frac{\partial \rho_r}{\partial A} \tag{54}$$

$$d_3 = \frac{\partial \rho_i}{\partial Q} - \frac{\rho_i}{\rho_r}\frac{\partial \rho_r}{\partial Q} \tag{55}$$

$$d_4 = \frac{\partial \rho_i}{\partial T_c} - \frac{\rho_i}{\rho_r}\frac{\partial \rho_r}{\partial T_c} \tag{56}$$

$$d_5 = \frac{\partial \rho_i}{\partial \Delta_c} - \frac{\rho_i}{\rho_r} \frac{\partial \rho_r}{\partial \Delta_c} \tag{57}$$

$$e_1 = \rho_i \frac{\partial \rho_i}{\partial P} + \rho_r \frac{\partial \rho_r}{\partial P} \tag{58}$$

$$e_2 = \rho_i \frac{\partial \rho_i}{\partial A} + \rho_r \frac{\partial \rho_r}{\partial A} \tag{59}$$

$$e_3 = \rho_i \frac{\partial \rho_i}{\partial Q} + \rho_r \frac{\partial \rho_r}{\partial Q} \tag{60}$$

$$e_4 = \rho_i \frac{\partial \rho_i}{\partial T_c} + \rho_r \frac{\partial \rho_r}{\partial T_c} \tag{61}$$

$$e_5 = \rho_i \frac{\partial \rho_i}{\partial \Delta_c} + \rho_r \frac{\partial \rho_r}{\partial \Delta_c} \tag{62}$$

and

$$k_2 = \rho_r + \frac{\rho_i^{\ 2}}{\rho_r} \tag{63}$$

$$k_3 = (1 + \rho_r^{\ 2} + \rho_i^{\ 2})\sqrt{(\rho_r^{\ 2} + \rho_i^{\ 2})}. \tag{64}$$

This gives the uncertainties in Δ and ψ for the conventional null ellipsometer as

$$\delta\Delta = \frac{1}{|k_2|} \left[|d_1\ \delta P| + |d_2\ \delta A| + |d_3\ \delta Q| + |d_4\ \delta T_c| + |d_5\ \delta\Delta_c| \right] \tag{65}$$

$$\delta\psi = \frac{1}{|k_3|} \left[|e_1\ \delta P| + |e_2\ \delta A| + |e_3\ \delta Q| + |e_4\ \delta T_c| + |e_5\ \delta\Delta_c| \right]. \tag{66}$$

The above equations are explicitly contained in the FORTRAN program which is described in the next section. These calculated uncertainties can be listed or plotted as a function of the angle of incidence, usually the one most easily varied ellipsometric parameter.

Program Description

The FORTRAN program which appears in the appendix of this report is described by the line numbers at the left-hand margin. In addition, a flow chart showing the program input and output data is given in figure 1. The program contains the introduction and declarations, line numbers 1 to 60; the places to enter in input data, line numbers 61 to

249; the theoretical calculations at every one degree of incident angle, line numbers 250 to 690; the program printout and graphics, lines numbers 691 to 757; and three short trigonometric subroutines. Except for the graphics subroutines for a Digital Equipment Corp. VAX-11 computer,* a FORTRAN IV or FORTRAN 77 compiler may be used for the program. A brief listing of some of the program line numbers with further explanation are as follows. The variables that need to be abbreviated or changed for the FORTRAN program are shown in parentheses.

Line Numbers	Description
69 to 75	choose between the bare- or film-substrate models
101 to 105	if bare substrate, film thickness is zero and
-	refractive index equals that of air
153 to 161	choose between entering conventional null data
-	or errors in Δ (DEL) and ψ (PSI)
248	defines substrate refractive index n_s (NS) in eq (12)
257	defines incident angle in radians, ϕ (PHI)
266	calculates eq (10) in text
283 to 286	calculates eqs (6), (7), (8), and (9)
303 to 304	calculates eqs (1), (2), (3), (4), and (5)
308 to 313	calculates Δ, ψ, and ρ (RHO) in eqs
-	(11), (26), and (27)
314	calculates ρ_c (RHOC) of the waveplate in eq (50)
333 to 340	calculate positions of the polarizer and analyzer at
-	null for zones one and three
410 to 424	$\delta\Delta$ (DDEL) and $\delta\psi$ (DPSI) are calculated for the null ellipsometer
-	case, eqs (63) and (64). In some variables
-	ρ_r (RHOR) and ρ_i (RHOI) are shortened to (RI) and (RR).
443 to 449	calculates $\frac{\partial\psi}{\partial t}$ (DPSIDT) and $\frac{\partial\Delta}{\partial t}$ (DDELDT) needed
-	in eqs (35) to (40)
506 to 513	calculates $\frac{\partial\psi}{\partial n_f}$ (DPSIDN) and $\frac{\partial\Delta}{\partial n_f}$ (DDELDN)
565 to 573	calculates $\frac{\partial\psi}{\partial\phi}$ (DPSIDO) and $\frac{\partial\Delta}{\partial\phi}$ (DDELDO)
596 to 603	calculates $\frac{\partial\psi}{\partial n_{sr}}$ (DPSDNR) and $\frac{\partial\Delta}{\partial n_{sr}}$ (DDEDNR)
626 to 633	calculates $\frac{\partial\psi}{\partial n_{si}}$ (DPSDNI) and $\frac{\partial\Delta}{\partial n_{si}}$ (DDEDNI)
636 to 640	calculates k_1 (K1) in eq (40)
644 to 661	calculates δt (DT) in eq (41) and δn_f (DNF) in eq (42)
665 to 691	calculates δn_{sr} (DNSR) and δn_{si} (DNSI) in eqs (24) and (25)

---

* Certain commercial equipment, instruments, or materials are identified in this paper in order to adequately specify the experimental procedure. Such identification does not imply recommendation or endorsement by the National Bureau of Standards, nor does it imply that the materials or equipment identified are necessarily the best available for the purpose.

See the program listing itself for the complete description.

Example Program Outputs

The following figures show how the uncertainties in refractive index and thickness vary with the angle of incidence. Figure 2 shows the uncertainties in refractive index and thickness for a 100-nm silicon dioxide film on silicon. There is relatively little angular variation for angles of incidence form 25 deg to 80 deg, and for uncertainties in the angle of incidence and Δ and ψ of 0.01 deg, the thickness and refractive index of the 100-nm film can be measured quite accurately. Figure 3 shows the variation of thickness and refractive index uncertainty for a thin 10-nm silicon dioxide film on silicon. Here, for uncertainties in the angle of incidence of 0.001 deg and Δ and ψ of 0.05 deg, the principal angle of incidence at 75.5 deg is the preferred angle of incidence to make the measurement. Figure 4 plots the uncertainties for a 280-nm silicon dioxide film thickness near the first order film-phase period occurring at about 70 deg. Although an accurate measurement cannot be made near 70 deg, one can still make a reasonably accurate measurement at an angle of incidence around 25 deg. Figure 5 plots for a silicon nitride film on silicon the uncertainties of thickness and refractive index. This differs from a silicon dioxide film in that its higher index, 1.98, gives rise to a more accurate measurement because of its index mismatch with air, and because the 80-nm silicon nitride film has its principal angle near 15 deg which is near the condition for maximum accuracy. Figure 6 shows how both the real and imaginary parts of the refractive index uncertainty vary as a function of the angle of incidence for the bare silicon substrate.

Conclusions

Many ellipsometers can make measurements to high precision. However, the present program allows one to calculate the maximum accuracy obtainable from any ellipsometer when performing an ellipsometric measurement using either one of two specific surface models: the refractive index of a bare substrate or the thickness and refractive index of a nonabsorbing film on a substrate. By inputting the appropriate uncertainties in the known measurement parameters, the maximum accuracy as a function of the angle of incidence can be displayed. By changing the magnitude of the input uncertainties, one can ascertain which parameter uncertainties are contributing the most to overall measurement uncertainty. When measuring an unknown bare substrate or a film of unknown thickness, one or two iterations of the input parameters, such as the incident angle, are necessary to maximize the accuracy.

An ellipsometer is an instrument that can be used to measure either the absolute optical properties of a surface or relative changes in them. Although the concern here is only with the accuracy of an absolute ellipsometric determination of these properties, because of the nonlinear nature of the electromagnetic theory that describes the measurement process, even relative changes in a surface's optical properties can be subject to large measurement error. An example of this type of measurement would be the calculated change in film thickness as a function of some growth parameter in terms of changes in Δ and ψ.

Requests for this program on recorded medium should be addressed to the author.

Acknowledgments

The author wishes to thank George A. Candela for the many enlightening discussions on ellipsometric instrumentation and theory.

References

1. F.L. McCrackin, A Fortran Program For Analysis Of Ellipsometric Measurements, NBS Technical Note 479 (April 1969).

2. R.M.A. Azzam and N.M. Bashara, Ellipsometry and Polarized Light (North-Holland, New York, 1977), pp. 388-389.

3. D. Chandler-Horowitz, Ellipsometric Accuracy and the Principal Angle of Incidence, SPIE Vol. 342, Integrated Circuit Metrology (1982), pp. 122-123.

4. D. Chandler-Horowitz and G.A. Candela, On the Accuracy of Ellipsometric Thickness Determinations For Very Thin Films, Journal De Physique Colloque C10, Ellipsometry '83 (Dec. 1983), pp. c10-24.

5. R.M.A. Azzam and N.M. Bashara, Chapter 4.

6. J. Humlicek, Evaluation of Derivatives of Reflectance and Transmittance by Stratified Structures and Solution of the Reverse Problem of Ellipsometry, Optica Acta, 1983, vol. 30, no. 1, p. 102.

7. F.L. McCrackin, p. 23.

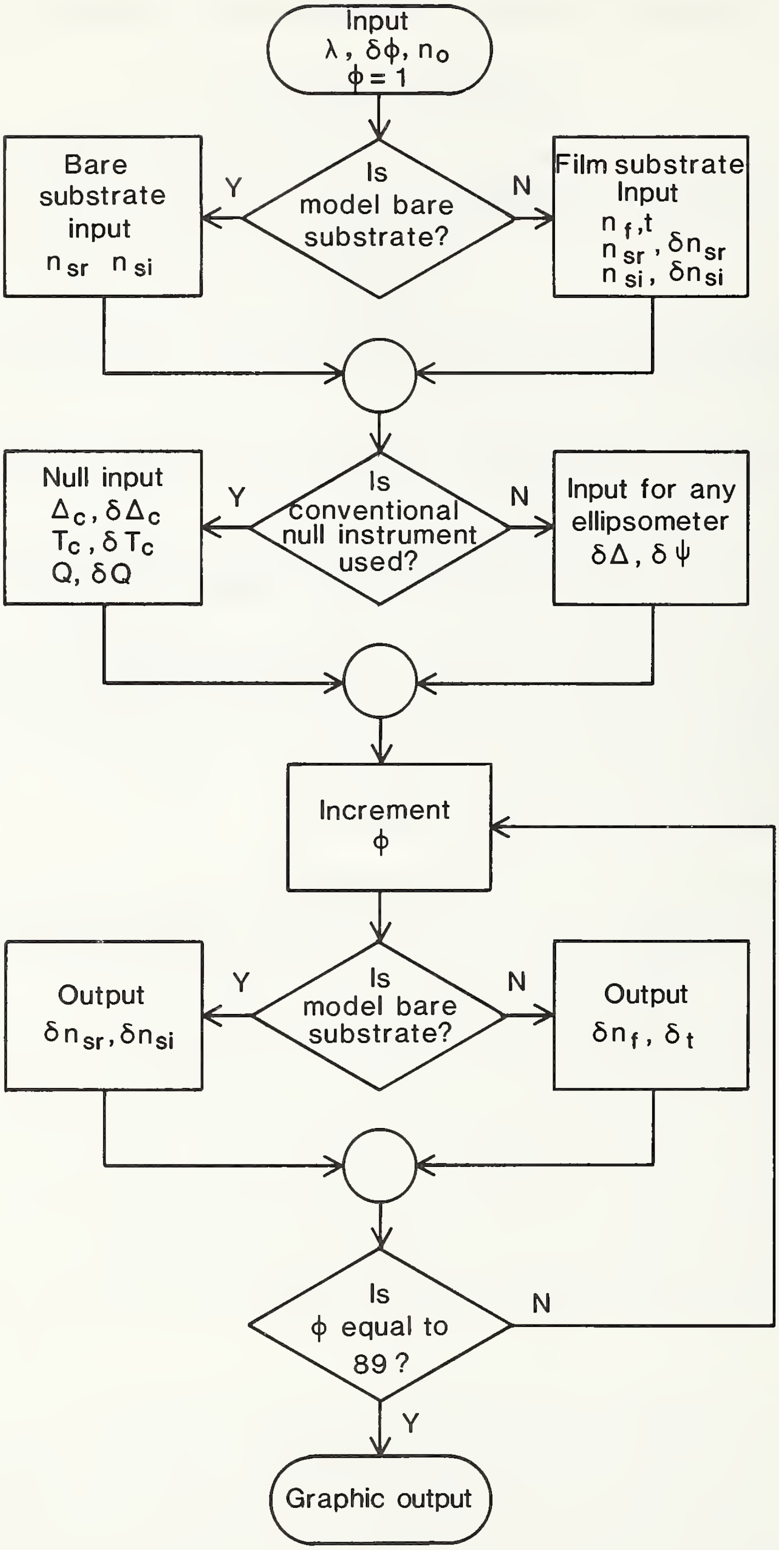


Figure 1. Program flow chart.

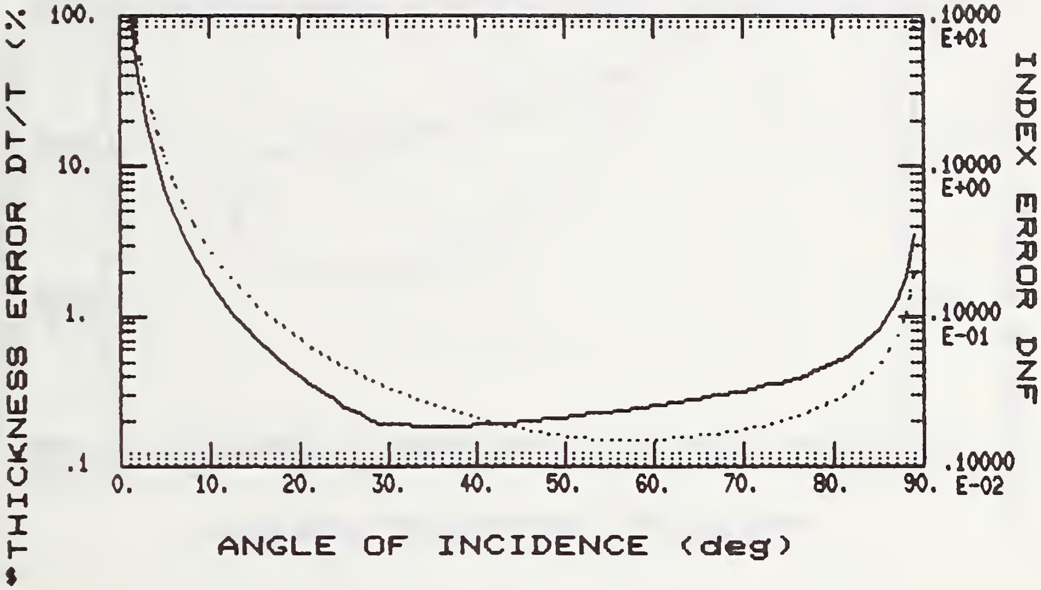


Figure 2. Plot of percent error of thickness (DT/T), solid line, and error in refractive index, dashed line, for an oxide film 100 nm thick on a silicon substrate. The input parameters are:

wavelength	632.8 nm
incident angle uncertainty	0.01 deg
film refractive index	1.46
film thickness	100 nm
substrate refractive index (real part)	3.865
uncertainty in real part	0.005
substrate refractive index (imag part)	0.018
uncertainty in imag part	0.002
uncertainty in DEL	0.05
uncertainty in PSI	0.05

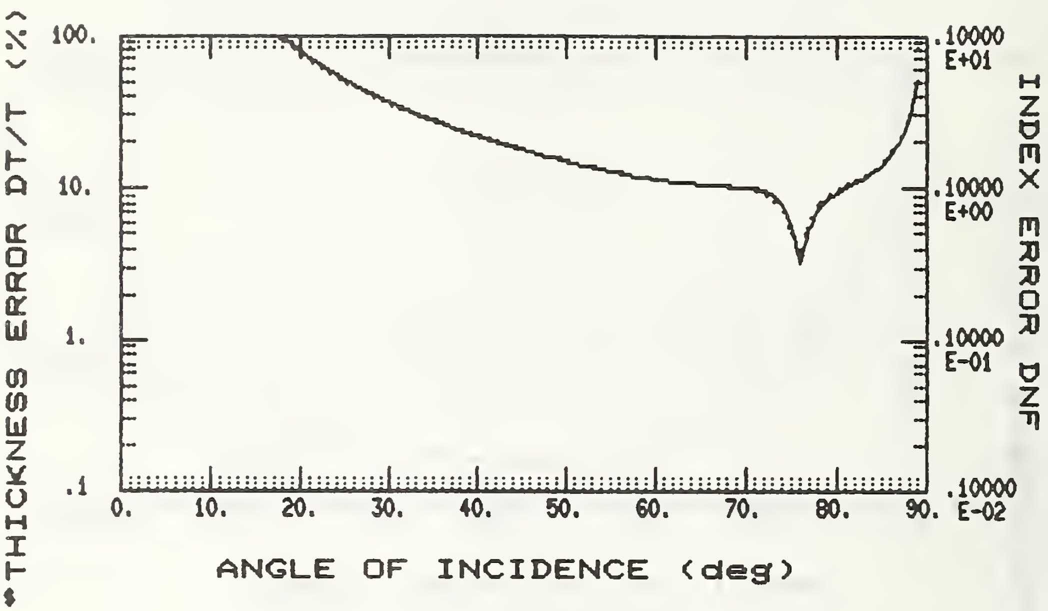


Figure 3. Plot of percent error in thickness (DT/T), solid line, and error in refractive index, dashed line, for an oxide film 10 nm thick on a silicon substrate. The input parameters are:

wavelength	632.8 nm
incident angle uncertainty	0.001 deg
film refractive index	1.46
film thickness	10 nm
substrate refractive index (real part)	3.865
uncertainty in real part	0.001
substrate refractive index (imag part)	0.018
uncertainty in imag part	0.001
uncertainty in DEL	0.02
uncertainty in PSI	0.02

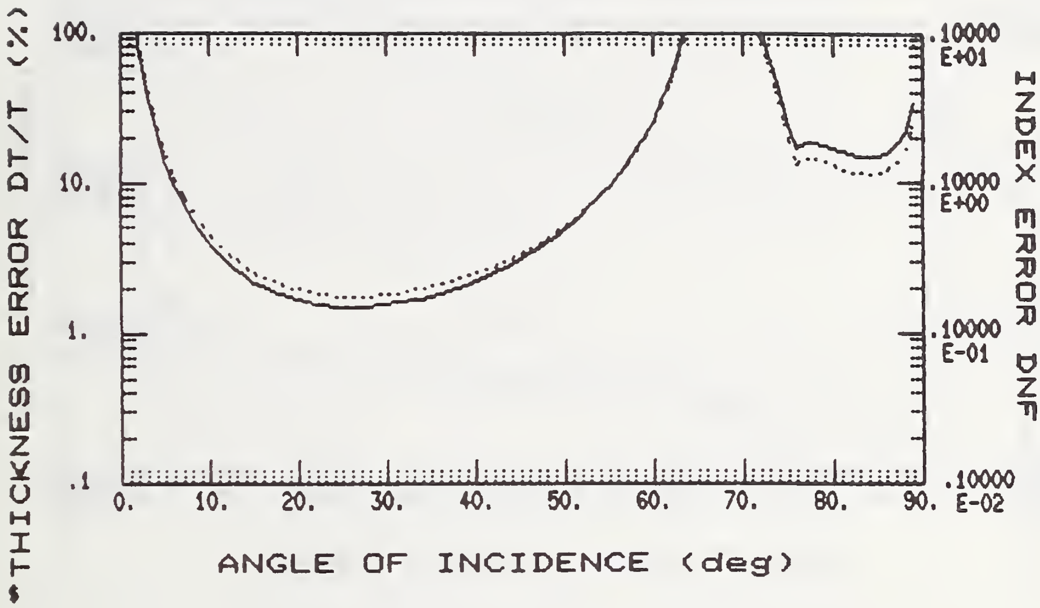


Figure 4. Plot of percent error of thickness (DT/T), solid line, and error in refractive index, dashed line, for an oxide film 280 nm thick on a silicon substrate. The input parameters are:

wavelength	632.8 nm
incident angle uncertainty	0.002 deg
film refractive index	1.46
film thickness	280 nm
substrate refractive index (real part)	3.865
uncertainty in real part	0.005
substrate refractive index (imag part)	0.018
uncertainty in imag part	0.002
uncertainty in DEL	0.02
uncertainty in PSI	0.02

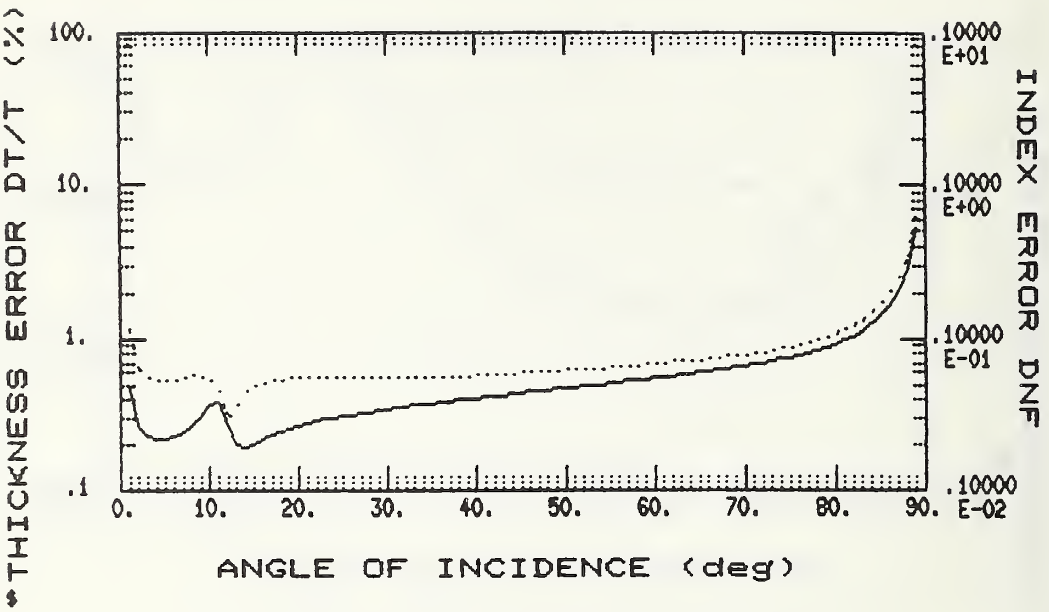


Figure 5. Plot of percent error of thickness (DT/T), solid line, and error in refractive index, dashed line, for a silicon nitride film 80 nm thick on a silicon substrate. The input parameters are:

wavelength	632.8 nm
incident angle uncertainty	0.01 deg
film refractive index	1.98
film thickness	80 nm
substrate refractive index (real part)	3.865
uncertainty in real part	0.005
substrate refractive index (imag part)	0.018
uncertainty in imag part	0.002
uncertainty in DEL	0.05
uncertainty in PSI	0.05

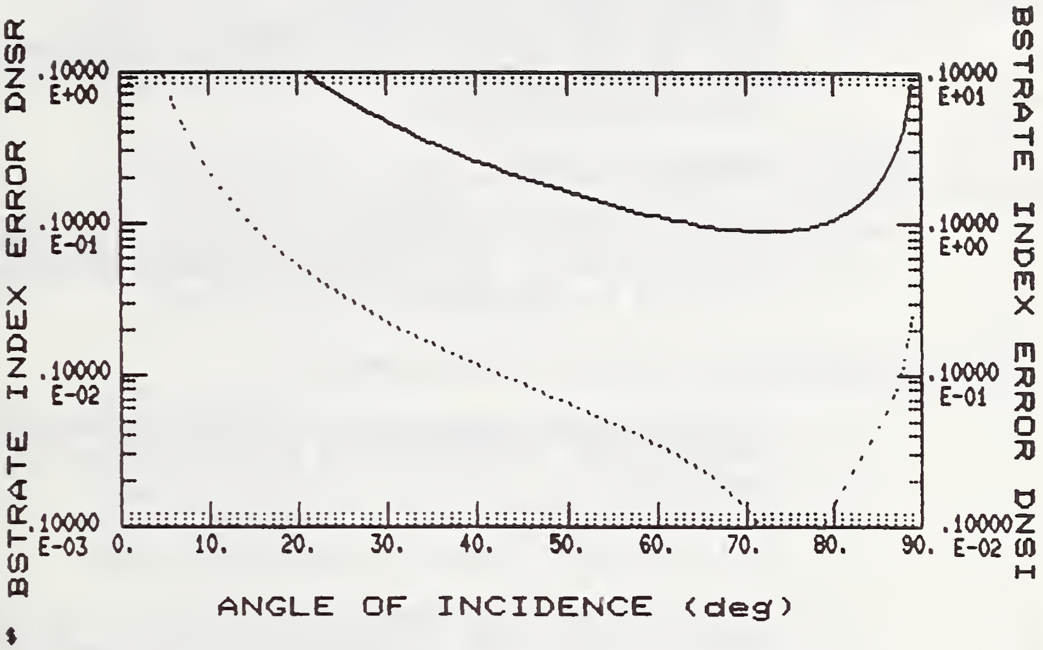


Figure 6. Plot of error in the refractive index (real part), solid line, and error in refractive index (imag part), dashed line, for a bare silicon substrate. The input parameters are:

wavelength	632.8 nm
incident angle uncertainty	0.01 deg
substrate refractive index (real part)	3.865
uncertainty in real part	0.005
substrate refractive index (imag part)	0.018
uncertainty in imag part	0.002
uncertainty in DEL	0.05
uncertainty in PSI	0.05

APPENDIX

```
C         PROGRAM         ERROR.FOR
C
C         WRITTEN BY DEANE CHANDLER-HOROWITZ
C                 NATIONAL BUREAU OF STANDARDS
C                 SEMICONDUCTOR MATERIALS AND PROCESSING DIVISION  725
C                 BLDG. 225, RM. A331
C                 GAITHERSBURG, MD 20899
C
C         DATE:   NOVEMBER 19, 1984
C
C         PURPOSE: TO CALCULATE THE UNCERTAINTY IN THE ELLIPSOMETRIC
C                 DETERMINATION OF THE THICKNESS AND INDEX OF REFRACTION
C                 OF A FILM ON A SUBSTRATE
C
C                                         OR
C
C                 TO CALCULATE THE UNCERTAINTY IN THE ELLIPSOMETRIC
C                 DETERMINATION OF THE INDEX OF REFRACTION OF A BARE
C                 SUBSTRATE
C
C                 AS A FUNCTION OF ANGLE OF INCIDENCE
C
C                 ASSUME THE AMBIENT-FILM-SUBSTRATE MODEL OR THE BARE
C                 SUBSTRATE MODEL BEST DESCRIBES THE ACTUAL SURFACE
C
C                 GIVEN THE UNCERTAINTIES IN THE ANGLE OF INCIDENCE,
C                 DEL AND PSI (OR IN THE CASE OF THE NULL ELLIPSOMETER,
C                 NULL VALUES OF POLARIZER AND ANALYSER, WAVEPLATE ANGLE,
C                 AND WAVEPLATE CONSTANTS), AND FOR THE BARE SUBSTRATE
C                 MODEL THE SUBSTRATE'S REFRACTIVE INDEX
C
C                 ASSUME NO WAVELENGTH UNCERTAINTY
C
C                 THIS PROGRAM VERSION CONTAINS EXPLICIT EXPRESSIONS FOR THE
C                 PARTIAL DERIVATIVES OF DEL AND PSI.
C
C-----------------------------------------------------------------------
C          MAKE NEEDED DECLARATIONS
C
        REAL Q,NF,NSR,NSI,NO,X(91),YT(91),YN(91),K1
C
        COMPLEX NS,CS,CRPFS,CRSFS,RP,RS,UP2,VP2,US2,VS2,EJ,AP,BP,AS,BS,
     1 DAPDT,DBPDT,DASDT,DBSDT,DRPDT,DRSDT,CT,QC,UP2DNF,VP2DNF,CPFSDN,
     2 CSFSDN,Z1,Z2,DAPDNF,DBPDNF,DASDNF,DBSDNF,DRPDNF,DRSDNF,CNF,UP2DO,
     3 VP2DO,CPFSDO,US2DO,VS2DO,CSFSDO,Y1,Y2,Y3,Y4,DAPDO,DBPDO,DASDO,
     4 DBSDO,DRPDO,DRSDO,CO,Z,RHO,RHOC,US2DNF,VS2DNF,US2DNR,VS2DNR,
     5 UP2DNR,VP2DNR,US2DNI,VS2DNI,UP2DNI,VP2DNI,CPFDNI,CPFDNR,CSFDNI,
     6 CSFDNR,DAPDNR,DAPDNI,DASDNR,DASDNI,DBSDNI,DBSDNR,DBPDNR,DBPDNI,
     7 ZA,ZB,ZC,ZD
C
        LOGICAL Q1
C
```

```
        WRITE (6,10)
10      FORMAT(1X,'THIS PROGRAM, ''ERROR.FOR'', CALCULATES THE
      1 UNCERTAINTY IN THE FILM')
        WRITE (6,20)
20      FORMAT(1X,'THICKNESS AND REFRACTIVE INDEX OR SUBSTRATE INDEX
      1 VERSUS INCIDENT ANGLE AS')
        WRITE (6,30)
30      FORMAT(1X,'FUNCTION OF THE EXPERIMENTAL ERRORS'/)
C
C       ----------------------------------------------------------------
C         ASK THE OPERATOR  FOR VALUES FOR PSI,DEL,WAVELENGTH,ANGLE OF
C            INCIDENCE,NO,NF,NS, AND THEIR UNCERTAINTIES
C
        RD=57.29578
C           CONVERTS DEGREES TO RADIANS
C
C                   CHOOSE BETWEEN THE BARE OR FILM-SUBSTRATE MODEL
        WRITE (6,40)
40      FORMAT(1X,'ENTER 1 FOR BARE SUBSTRATE')
        WRITE (6,50)
50      FORMAT(1X,'ENTER 2 FOR FILM-SUBSTRATE')
        READ (5,60) II
60      FORMAT(I1)
C
C                   ENTER INPUT DATA
C
        IF (II .EQ. 1) WRITE (4,70)
70      FORMAT(T30,'SUBSTRATE REFRACTIVE INDEX UNCERTAINTY'/)
        IF (II .EQ. 2) WRITE (4,80)
80      FORMAT(T30,'FILM INDEX AND THICKNESS UNCERTAINTY'/)
C
        WRITE(4,90)
        WRITE(6,90)
90      FORMAT(1X,'ENTER WAVELENGTH IN NANOMETERS')
        READ(5,100) WL
        WRITE(4,100) WL
100     FORMAT(F10.2)
C
        WRITE(4,110)
        WRITE(6,110)
110     FORMAT(/1X,'ENTER UNCERTAINY IN ANGLE OF INCIDENCE IN DEGREES')
        READ(5,120) DPHI
        WRITE(4,120) DPHI
120     FORMAT(F10.3)
        DPHI=DPHI/RD
C
        NO=1.00036
C          INDEX OF AIR
C                       IF BARE SUBSTRATE, FILM THICKNESS IS ZERO AND
C                       REFRACTIVE INDEX EQUALS THAT OF AIR
C
125     IF (II .EQ. 1) NF=NO
```

```
      IF (II .EQ. 1) T=0
126   IF (II .EQ. 1) GOTO 170
      WRITE(4,130)
      WRITE(6,130)
130   FORMAT(/1X,'ENTER INDEX OF REFRACTION OF FILM (NON-ABSORBING)')
      READ(5,140) NF
      WRITE(4,140) NF
140   FORMAT(F9.4)
C
      WRITE(4,150)
      WRITE(6,150)
150   FORMAT(/1X,'ENTER THICKNESS OF FILM IN NANOMETERS')
      READ(5,160) T
      WRITE(4,160) T
160   FORMAT(F10.2)
C
170   WRITE(4,180)
      WRITE(6,180)
180   FORMAT(/1X,'ENTER REAL PART OF SUBSTRATE REFRACT INDEX')
      READ(5,190) NSR
      WRITE(4,190) NSR
190   FORMAT(F9.4)
C
      IF (II .EQ. 1) GOTO 220
      WRITE(4,200)
      WRITE(6,200)
200   FORMAT(/1X,'ENTER UNCERTAINTY IN REAL PART OF SUBSTRATE
     1 REFRACTIVE INDEX')
      READ(5,210) DNSR
      WRITE(4,210) DNSR
210   FORMAT(F9.4)
C
220   WRITE(4,230)
      WRITE(6,230)
230   FORMAT(/1X,'ENTER IMAGINARY PART OF SUBSTRATE REFRACT INDEX')
      READ(5,240) NSI
      WRITE(4,240) NSI
240   FORMAT(F9.4)
C
      IF (II .EQ. 1) GOTO 270
      WRITE(4,250)
      WRITE(6,250)
250   FORMAT(/1X,'ENTER UNCERTAINTY IN IMAGINARY PART OF SUBSTRATE
     1 REFRACTIVE INDEX')
      READ(5,260) DNSI
      WRITE(4,260) DNSI
260   FORMAT(F9.4)
C
C                      CHOOSE BETWEEN ENTERING CONVENTIONAL NULL DATA
C                      OR ERRORS IN DEL AND PSI
C
270   WRITE(6,280)
```

```
  280 FORMAT(/1X,'DO YOU HAVE NULL DATA AVAILABLE? (T/F)')
      READ(5,290) Q1
  290 FORMAT(L1)
C
      IF (Q1 .EQ. .FALSE.) GOTO 460
      WRITE(4,300)
      WRITE(6,300)
  300 FORMAT(/1X,'ENTER  UNCERTAINY FOR POLARIZER NULL IN DEGREES')
      READ(5,310) DP
      WRITE(4,310) DP
  310 FORMAT(F9.3)
      DP=DP/RD
C
      WRITE(4,320)
      WRITE(6,320)
  320 FORMAT(/1X,'ENTER UNCERTAINY FOR ANALYSER NULL IN DEGREES')
      READ(5,330) DA
      WRITE(4,330) DA
  330 FORMAT(F9.3)
      DA=DA/RD
C
      WRITE(4,340)
      WRITE(6,340)
  340 FORMAT(/1X,'ENTER THE WAVEPLATE RETARDATION IN DEGREES')
      READ(5,350) DELC
      WRITE(4,350) DELC
  350 FORMAT(F9.3)
      DELC=DELC/RD
C
      WRITE(4,360)
      WRITE(6,360)
  360 FORMAT(/1X,'ENTER THE WAVEPLATE RETARDATION UNCERTAINTY IN
     1 DEGREES')
      READ(5,370) DDELC
      WRITE(4,370) DDELC
  370 FORMAT(F9.3)
      DDELC=DDELC/RD
C
      WRITE(4,380)
      WRITE(6,380)
  380 FORMAT(/1X,'ENTER THE WAVEPLATE TRANSMISSION COEFF.')
      READ(5,390) TC
      WRITE(4,390) TC
  390 FORMAT(F10.5)
C
      WRITE(4,400)
      WRITE(6,400)
  400 FORMAT(/1X,'ENTER THE WAVEPLATE TRANS. COEFF. UNCERTAINTY')
      READ(5,410) DTC
      WRITE(4,410) DTC
  410 FORMAT(F10.5)
C
```

```
      WRITE(4,420)
      WRITE(6,420)
420   FORMAT(/1X,'ENTER THE WAVEPLATE AZIMUTH ANGLE (ie +-45 deg)')
      READ(5,430) Q
      WRITE(4,430) Q
430   FORMAT(F9.3)
      Q=Q/RD
C
      WRITE(4,440)
      WRITE(6,440)
440   FORMAT(/1X,'ENTER THE WAVEPLATE AZIMUTH ANGLE UNCERTAINTY
     1  IN DEGREES')
      READ(5,450) DQ
      WRITE(4,450) DQ
450   FORMAT(F9.3)
      DQ=DQ/RD
C
C
       GOTO 1000
C
C              ERRORS IN DEL AND PSI GIVEN
460   WRITE(4,470)
      WRITE(6,470)
470   FORMAT(/1X,'ENTER UNCERTAINTY IN DEL IN DEGREES')
      READ(5,480) DDEL
      WRITE(4,480) DDEL
480   FORMAT(F10.3)
      DDEL=DDEL/RD
C
      WRITE(4,490)
      WRITE(6,490)
490   FORMAT(/1X,'ENTER UNCERTAINTY IN PSI IN DEGREES')
      READ(5,500) DPSI
      WRITE(4,500) DPSI
500   FORMAT(F10.3)
      DPSI=DPSI/RD
C
C     REFRACTIVE INDEX OF SUBSTRATE, NS AS IN EQUATION (12)
C
1000  NS=CMPLX(NSR,-NSI)
C
C     ----------------------------------------------------------------
C        BEGIN LOOP FOR ALL ANGLES OF INCIDENCE, EVERY DEGREE
C
      DO 5000 I=1,89
C
C                INCIDENT ANGLE IN RADIANS, PHI
C
      PHI=I/RD
      SO=SIN(PHI)
      CO=COS(PHI)
      YY=NO*SO
      CF=SQRT(1.-(YY/NF)**2)
      CS=CSQRT(1.-(YY/NS)**2)
C
        DEFINE BETA,B AS IN EQUATION (10)
C
      B=8.*ATAN(1.)*T/WL*NF*CF
C
        CALC FRESNEL EQUATIONS
          BREAK UP INTO SMALLER PIECES
C
      UP1=NF*CO-NO*CF
      VP1=NF*CO+NO*CF
      UP2=NS*CF-NF*CS
      VP2=NS*CF+NF*CS
      US1=NO*CO-NF*CF
      VS1=NO*CO+NF*CF
      US2=NF*CF-NS*CS
      VS2=NF*CF+NS*CS
C
C              CALC THE FRESNEL COEFFICIENTS RPOF AND RSOF, EQS.
C              (6) AND (7) AND CRPFS AND CRSFS IN EQS. (8) AND (9)
C
      RPOF=UP1/VP1
      CRPFS=UP2/VP2
      RSOF=US1/VS1
      CRSFS=US2/VS2
C
C       DEFINE EJ, IMAGINARY EXPONENT E TO THE -2*B
C
      Z=CMPLX(0.,-2.*B)
      EJ=CEXP(Z)
C
C
C
      AP=RPOF+CRPFS*EJ
      BP=1+RPOF*CRPFS*EJ
      AS=RSOF+CRSFS*EJ
      BS=1+RSOF*CRSFS*EJ
C
C       CALC RP AND RS FOR THE BARE SUBSTRATE MODEL, EQS. (2),(3)
C       AND FOR THE FILM-SUBSTRATE MODEL, EQS. (4) AND (5)
C
      RP=AP/BP
      RS=AS/BS
C
C       CALC DEL AND PSI FROM INPUT PARAMETERS
C
      PSI=ATAN(CABS(RP/RS))
      DEL=ATAN2(AIMAG(RP/RS),REAL(RP/RS))
C
C              DEFINITION OF RHO, RP/RS AS IN EQUATION (1)
C
```

```
      RHO=RP/RS
      RHOC=TC*CEXP((0.,-1.)*DELC)
C
C     ---------------------------------------------------------------
C      IF ERRORS IN DEL AND PSI GIVEN JUMP AHEAD
      IF (Q1 .EQ. .FALSE.) GOTO 1150
C
C       FOR CONVENTIONAL NULL ELLISOMETER CALCULATE NULL CONDITIONS
C       FOR ZONE 1 -- BEGIN CALC FOR DDEL AND DPSI
C
      IF(ABS(DEL) .LT. 1.0E-8) GOTO 1100
      R=(TAN(Q)*SIN(DEL-DELC)-SIN(DEL+DELC)/TAN(Q))/2./SIN(DEL)
C
      TP1=(-R+SQRT(R*R+1))/TC
      TP2=(-R-SQRT(R*R+1))/TC
      P1=ATAN(TP1)+Q
      P3=ATAN(TP2)+Q
      A1=ATAN(REAL(RHO*(TP1*TAN(Q)*RHOC-1.)/(TAN(Q)+TP1*RHOC)))
      A3=ATAN(REAL(RHO*(TP2*TAN(Q)*RHOC-1.)/(TAN(Q)+TP2*RHOC)))
      GOTO 1110
 1100 P1=Q
      P3=Q-90./RD
      A1=ATAN(REAL(RHO/TAN(Q)))
      A3=ATAN(REAL(RHO*TAN(Q)))
 1110 P1=AMOD(P1+360./RD,180./RD)
      A1=AMOD(A1+360./RD,180./RD)
      P3=AMOD(P3+360./RD,180./RD)
      A3=AMOD(A3+360./RD,180./RD)
C
C                AND NOW FOR THE ERRORS IN DEL AND PSI
C      ZONE 1
      P=P1
      A=A1
C
C       DEFINE QUARTER-WAVE PLATE AZIMUTH ANGULAR QUANTITIES
C
      TQ=TAN(Q)
      TQ2=TAN(Q)*TAN(Q)
      TPQ=TAN(P-Q)
      TPQ2=TAN(P-Q)*TAN(P-Q)
      SQ=SEC(Q)
      SQ2=SEC(Q)*SEC(Q)
      SPQ=SEC(P-Q)
      SPQ2=SEC(P-Q)*SEC(P-Q)
C
C       CALC RHOR AND RHOI AS IN EQN. (31)
C
      DD=TC*TC*TQ2*TPQ2+1+2.*TC*TQ*TPQ*COS(DELC)
      RHOR=(TAN(A)/DD)*(-TQ+TC*TC*TQ*TPQ2+TQ2*TC*TPQ*COS(DELC)
     1 -TC*TPQ*COS(DELC))
      RHOI=(TAN(A)/DD)*(-TQ2*TC*TPQ*SIN(DELC)-TC*TPQ*SIN(DELC))
C
```

```
C        CALC ALL PARTIAL DERIVATIVES NEEDED IN EQNS. (33) AND (34)
C
C        DRRDA=dRHOR/dA,DRIDA=dRHOI/dA
C
      DRRDA=2.*RHOR/SIN(2.*A)
      DRIDA=2.*RHOI/SIN(2.*A)
C
C        DRRDP=dRHOR/dP,DRIDP=dRHOI/dP
C
      DRRDP=TAN(A)*SPQ2*TC*(TC*TQ*2.*TPQ+COS(DELC)*(TQ2-1.))/DD
      DRRDP=DRRDP-RHOR*2.*SPQ2*TQ*TC*(TC*TQ*TPQ+COS(DELC))/DD
      DRIDP=TAN(A)*SIN(DELC)*TC*SPQ2*(-TQ-1.)/DD
      DRIDP=DRIDP-RHOI*2.*SPQ2*TQ*TC*(TC*TQ*TPQ+COS(DELC))/DD
C
C       DRRDQ=dRHOR/dQ,DRIDQ=dRHOI/dQ
C
      DRRDQ=TAN(A)*(-SQ2+TC*TC*(SQ2*TPQ2-TQ*2.*TPQ*SPQ2)+TC
     1 *COS(DELC)*(2.*TQ*SQ2*TPQ-TQ2*SPQ2)+TC*SPQ2*COS(DELC))/DD
      DRRDQ=DRRDQ-RHOR*(TC*TC*(2.*TQ*SQ2*TPQ2-2.*TQ2*TPQ*SPQ2)+
     1 2.*TC*COS(DELC)*(SQ2*TPQ-TQ*SPQ2))/DD
C
      DRIDQ=TAN(A)*SIN(DELC)*TC*(-2.*TQ*SQ2*TPQ+TQ2*SPQ2+SPQ2)/DD
      DRIDQ=DRIDQ-RHOI*(TC*TC*(2.*TQ*SQ2*TPQ2-2.*TQ2*TPQ*SPQ2)+2.*TC*
     1 COS(DELC)*(SQ2*TPQ-TQ*SPQ2))/DD
C
C        DRRDTC=dRHOR/dTC,DRIDTC=dRHOI/dTC
C
      DRRDTC=TAN(A)*(2.*TC*TQ*TPQ2+TQ2*TPQ*COS(DELC)-TPQ*COS(DELC))
     1 /DD-RR*(2.*TC*TQ2*TPQ2+2.*TQ*TPQ*COS(DELC))/DD
C
      DRIDTC=TAN(A)*(-TQ2*TPQ*SIN(DELC)-TPQ*SIN(DELC))/DD-RHOI*(2.*
     1 TC*TQ2*TPQ2+2.*TQ*TPQ*COS(DELC))/DD
C
C        DRRDDC=dRHOR/dDELC,DRIDDC=dRHOI/dDELC
C
      DRRDDC=-TAN(A)*SIN(DELC)*(TQ2*TC*TPQ-TC*TPQ)/DD+RHOR*SIN(DELC)
     1 *2.*TC*TQ*TPQ/DD
C
      DRIDDC=-TAN(A)*COS(DELC)*(TQ2*TC*TPQ+TC*TPQ)/DD+RHOI*SIN(DELC)
     1 *2.*TC*TQ*TPQ/DD
C
C        DDEL=dDEL, DPSI=dPSI AS IN EQNS. (33) AND (34) DUE TO ERRORS
C        IN THE QUARTER-WAVE PLATE AND POLARIZER AND ANALYSER NULL
C        POSITIONS FOR THE CONVENTIONAL NULL ELLIPSOMETRIC METHOD.
C
      DDEL=(DRIDP-RHOI*DRRDP/RHOR)**2*DP*DP
      DDEL=DDEL+(DRIDA-RHOI*DRRDA/RHOR)**2*DA*DA
      DDEL=SQRT(DDEL)
      DDEL=DDEL+ABS(DRIDQ-RHOI*DRRDQ/RHOR)*DQ
      DDEL=DDEL+ABS(DRIDTC-RHOI*DRRDTC/RHOR)*DTC
      DDEL=DDEL+ABS(DRIDDC-RHOI*DRRDDC/RHOR)*DDELC
      DDEL=1/ABS(RHOR)/(1+RHOI*RHOI/RHOR/RHOR)*DDEL
```

```
C
       DPSI=(RHOI*DRIDP+RHOR*DRRDP)**2*DP*DP
       DPSI=DPSI+(RHOI*DRIDA+RHOR*DRRDA)**2*DA*DA
       DPSI=SQRT(DPSI)
       DPSI=DPSI+ABS(RHOI*DRIDQ+RHOR*DRRDQ)*DQ
       DPSI=DPSI+ABS(RHOI*DRIDTC+RHOR*DRRDTC)*DTC
       DPSI=DPSI+ABS(RHOI*DRIDDC+RHOR*DRRDDC)*DDELC
       DPSI=1/(1+RHOR*RHOR+RHOI*RHOI)/SQRT(RHOR*RHOR+RHOI*RHOI)*DPSI
C
C      -------------------------------------------------------------------
1150   CONTINUE
C          COME HERE FOR DEL,PSI ERROR INPUT
       IF (II .EQ. 1) GOTO 1300
C
C             BEGIN UNCERTAINTY CALC HERE FOR FILM-SUBSTRATE MODEL
C
C        CALC PARTIAL DIFFERENTIALS OF B,AP,BP,AS,BS WITH RESPECT TO T
C        DBDT=dB/dT,DAPDT=dAP/dT,DBPDT=dBP/dT,DASDT=dAS/dT,DBSDT=dBS/dT
C
       DBDT=8.*ATAN(1.)/WL*NF*CF
       DAPDT=-2.*(0.,1.)*CRPFS*EJ*DBDT
       DBPDT=-2.*(0.,1.)*RPOF*CRPFS*EJ*DBDT
       DASDT=-2.*(0.,1.)*CRSFS*EJ*DBDT
       DBSDT=-2.*(0.,1.)*RSOF*CRSFS*EJ*DBDT
C
C
C        CALC PARTIAL DIFFERENTIALS OF PSI AND DEL WITH RESPECT TO T
C        DPSIDT=dPSI/dT,DDELDT=dDEL/dT AS IN EQNS (22) AND (23)
C
       DPSIDT=SIN(2.*PSI)/2.*REAL(DAPDT/AP+DBSDT/BS-
     1 DASDT/AS-DBPDT/BP)
C
       DDELDT=AIMAG(DAPDT/AP+DBSDT/BS-DASDT/AS-DBPDT/BP)
C
C        CALC PARTIAL DIFFERENTIALS OF RP, RS AND B WITH RESPECT TO NF
C
C        FIRST DEFINE P AND QC TO HELP WITH CALCULATIONS
C
       P=SQRT(NF*NF-NO*NO*SO*SO)
       QC=CSQRT(NS*NS-NO*NO*SO*SO)
C
C        CALC PARTIAL OF B WITH RESPECT TO NF
C        DBDNF=dB/dNF
C
       DBDNF=B/NF/CF/CF
C
C        CALC PARTIAL DIFFERENTIALS OF RPOF, CRPFS, RSOF, CRSFS
C        UP1DNF=dUP1/dNF,VP1DNF=dVP1/dNF,DUP2DNF=dUP2/dNF,DVP2DNF=dVP2/dNF
C
       UP1DNF=CO-NO**3*SO*SO/NF**2/P
       VP1DNF=CO+NO**3*SO*SO/NF**2/P
       UP2DNF=NS*NO*NO*SO*SO/NF**2/P-CS
```

```
      VP2DNF=NS*NO*NO*SO*SO/NF**2/P+CS
C
C       PARTIAL DIFFERENTIAL OF RP01 AND CRPFS WITH RESPECT TO NF
C       RPOFDN=dRPOF/dNF,CPFSDN=dCRPFS/dNF
C
      RPOFDN=UP1DNF/VP1-VP1DNF*UP1/VP1/VP1
      CPFSDN=UP2DNF/VP2-VP2DNF*UP2/VP2/VP2
C
C       US1DNF=dUS1/dNF,VS1DNF=dVS1/dNF,US2DNF=dUS2/dNF,DVS2DNF=dVS2/dNF
C
      US1DNF=-NF/P
      VS1DNF=NF/P
      US2DNF=NF/P
      VS2DNF=NF/P
C
C       ALL THE ABOVE PARTIALS ARE ALMOST THE SAME
C
C        PARTIALS OF RSOF AND CRSFS
C        RSOFDN=dRSOF/dNF,CSFSDN=dCRSFS/dNF
C
      RSOFDN=US1DNF/VS1*(1.+US1/VS1)
      CSFSDN=US2DNF/VS2*(1.-US2/VS2)
C
C       NOW GET THE PARTIALS OF AP,BP,AS,BS
C       DAPDNF=dAP/dNF,DBPDNF=dBP/dNF
C
      Z1=2.*(0.,1.)*CRPFS*EJ*DBDNF
      DAPDNF=RPOFDN+EJ*CPFSDN-Z1
      DBPDNF=EJ*(RPOF*CPFSDN+CRPFS*RPOFDN-RPOF*Z1/EJ)
C
C       DASDNF=dAS/dNF,DBSDNF=dBS/dNF
C
      Z2=2.*(0.,1.)*CRSFS*EJ*DBDNF
      DASDNF=RSOFDN+EJ*CSFSDN-Z2
      DBSDNF=EJ*(RSOF*CSFSDN+CRSFS*RSOFDN-RSOF*Z2/EJ)
C
C
C       PARTIAL DIFFERENTIALS OF PSI AND DEL WITH RESPECT TO NF
C       AS IN EQNS. (21) AND(23)
C       DPSIDN=dPSI/dNF,DDELDN=dDEL/dNF
C
      DPSIDN=SIN(2.*PSI)/2.*REAL(DAPDNF/AP+DBSDNF/BS-
     1 DASDNF/AS-DBPDNF/BP)
      DDELDN=AIMAG(DAPDNF/AP+DBSDNF/BS-DASDNF/AS-
     1 DBPDNF/BP)
C
C
C       DEFINE ALL PARTIAL DIFFERENTIALS WITH RESPECT TO PHI
C
C       PARTIAL DIFFERENTIAL OF B WITH RESPECT TO PHI
C       DBD0=dB/dPHI
C
```

```
      DBD0=-4.*NO*NO*T*ATAN(1.)/WL*SIN(2.*PHI)/P
C
C       PARTIALS OF RPOF,CRPFS WITH RESPECT TO PHI
C       UP1D0=dUP1/dPHI,VP1D0=dVP1/dPHI,UP2D0=dUP2/dPHI,VP2D0=dVP2/dPHI
C
      UP1D0=-NF*SO+NO**3*SIN(2.*PHI)/2./NF/P
      VP1D0=-NF*SO-NO**3*SIN(2.*PHI)/2./NF/P
      UP2D0=-NS*NO*NO*SIN(2.*PHI)/2./NF/P+NF*NO*NO*SIN(2.*PHI)/
     1 2./NS/QC
      VP2D0=-NS*NO*NO*SIN(2.*PHI)/2./NF/P-NF*NO*NO*SIN(2.*PHI)/
     1 2./NS/QC
C
C       RPOFD0=dRPOF/dPHI,CPFSD0=dCPFS/dPHI
C
      RPOFD0=UP1D0/VP1-VP1D0*UP1/VP1/VP1
      CPFSD0=UP2D0/VP2-VP2D0*UP2/VP2/VP2
C
C       PARTIALS OF RSOF AND CRSFS
C       US1D0=dUS1/dPHI,VS1D0=dVS1/dPHI,US2D0=dUS2/dPHI,VS2D0=dVS2/dPHI
C
      US1D0=-NO*SO+NO*NO*SIN(2.*PHI)/2./P
      VS1D0=-NO*SO-NO*NO*SIN(2.*PHI)/2./P
      US2D0=NO*NO*SIN(2.*PHI)/2.*(-1./P+1./QC)
      VS2D0=NO*NO*SIN(2.*PHI)/2.*(-1./P-1./QC)
C
C       RSOFD0=dRSOF/dPHI,CSFSD0=dCSFS/dPHI
C
      RSOFD0=US1D0/VS1-VS1D0*US1/VS1/VS1
      CSFSD0=US2D0/VS2-VS2D0*US2/VS2/VS2
C
C       PARTIALS OF AP,BP,AS, AND BS WITH RESPECT OF PHI
C       DAPD0=dAP/dPHI,DBPD0=dBP/dPHI,DASD0=dAS/dPHI,DBSD0=dBS/dPHI
C
      Y1=2.*(0.,1.)*CRPFS*EJ*DBD0
      DAPD0=RPOFD0+EJ*CPFSD0-Y1
      Y2=2.*(0.,1.)*CRPFS*RPOF*DBD0
      DBPD0=EJ*(CRPFS*RPOFD0+RPOF*CPFSD0-Y2)
      Y3=2.*(0.,1.)*CRSFS*EJ*DBD0
      DASD0=RSOFD0+EJ*CSFSD0-Y3
      Y4=2.*(0.,1.)*CRSFS*RSOF*DBD0
      DBSD0=EJ*(CRSFS*RSOFD0+RSOF*CSFSD0-Y4)
C
C       (PARTIALS OF RP AND RS WITH RESPECT TO PHI)
C
C       CALC PARTIAL DIFFERENTIALS OF PSI AND DELTA WITH RESPECT TO PHI
C       TRIG FUNCTIONS OF DEL AND PSI
C       AS IN EQNS. (21) AND (22)
C       DPSID0=dPSI/dPHI,DDELD0=dDEL/dPHI
C
      DPSID0=SIN(2.*PSI)/2.*REAL(DAPD0/AP+DBSD0/BS-
     1 DASD0/AS-DBPD0/BP)
      DDELD0=AIMAG(DAPD0/AP+DBSD0/BS-
     1 DASDO/AS-DBPDO/BP)
C
C        TAKE DERIVATIVES WITH RESPECT TO THE REAL PART OF THE
C        SUBSTRATE REFRACTIVE INDEX, NSR
C        UP2DNR=dUP2/dNSR,VP2DNR=dVP2/dNSR,US2DNR=dUS2/dNSR,VS2DNR=dVS2/dNSR
C
      UP2DNR=CF+NF*YY*YY/(NS**3)/CS
      VP2DNR=CF-NF*YY*YY/(NS**3)/CS
      US2DNR=-CS+YY*YY/(NS*NS*CS)
      VS2DNR=CS-YY*YY/(NS*NS*CS)
C
C        CPFDNR=dCRPFS/dNSR,CSFDNR=dCRSFS/dNSR
C
      CPFDNR=UP2DNR/VP2-VP2DNR*UP2/VP2/VP2
      CSFDNR=US2DNR/VS2*(1.+US2/VS2)
C
C        DAPDNR=dAP/dNSR,DBPDNR=dBP/dNSR,DASDNR=dAS/dNSR,DBSDNR=dBS/dNSR
C
      DAPDNR=EJ*CPFDNR
      DBPDNR=EJ*RPOF*CPFDNR
      DASDNR=EJ*CSFDNR
      DBSDNR=EJ*RSOF*CSFDNR
C
C        CALCULATE PARTIAL DERIVATIVES OF PSI AND DEL WITH RESPECT TO NSR
C        AS IN EQNS. (21) AND (22)
C        DPSDNR=dPSI/dNSR,DDEDNR=dDEL/dNSR
C
      DPSDNR=SIN(2.*PSI)/2.*REAL(DAPDNR/AP+DBSDNR/BS-
     1 DASDNR/AS-DBPDNR/BP)
      DDEDNR=AIMAG(DAPDNR/AP+DBSDNR/BS-DASDNR/AS-
     1 DBPDNR/BP)
C
C        TAKE DERIVATIVES WITH RESPECT TO THE IMAG PART OF THE
C        SUBSTRATE REFRACTIVE INDEX, NSI
C        UP2DNI=dUP2/dNSI,VP2DNI=dVP2/dNSI,US2DNI=dUS2/dNSI,VS2DNI=dVS2/dNSI
C
      UP2DNI=(CF+NF*YY*YY/(NS**3)/CS)*(0.,-1.)
      VP2DNI=(CF-NF*YY*YY/(NS**3)/CS)*(0.,-1.)
      US2DNI=(-CS+YY*YY/(NS*NS*CS))*(0.,-1.)
      VS2DNI=(CS-YY*YY/(NS*NS*CS))*(0.,-1.)
C
C        CPFDNI=dCRPFS/dNSI,CSFDNI=dCRSFS/dNSI
C
      CPFDNI=UP2DNI/VP2-VP2DNI*UP2/VP2/VP2
      CSFDNI=US2DNI/VS2*(1.+US2/VS2)
C
C        DAPDNI=dAP/dNSI,DBPDNI=dBP/dNSI,DASDNI=dAS/dNSI,DBSDNI=dBS/dNSI
C
      DAPDNI=EJ*CPFDNI
      DBPDNI=EJ*RPOF*CPFDNI
      DASDNI=EJ*CSFDNI
      DBSDNI=EJ*RSOF*CSFDNI
```

```
C
C         PARTIAL DERIVATIVES OF PSI AND DEL WITH RESPECT TO NSI
C         AS IN EQNS. (21) AND (22)
C         DPSDNI=dPSI/dNSI,DDEDNI=dDEL/dNSI
C
       DPSDNI=SIN(2.*PSI)/2.*REAL(DAPDNI/AP+DBSDNI/BS-
     1 DASDNI/AS-DBPDNI/BP)
       DDEDNI=AIMAG(DAPDNI/AP+DBSDNI/BS-DASDNI/AS-
     1 DBPDNI/BP)

C
C         FINALLY DEFINE PARTIAL OF NF, THICKNESS  DENOMINATOR TERM
C         AS IN EQN. (23)
C
C
       K1=ABS(DPSIDN*DDELDT-DDELDN*DPSIDT)
C
       IF (K1 .EQ. 0) K1=1.0E-35
C
C         FINAL RESULT OF SUMS IN EQNS. (21) AND (22)
C
       DET1=ABS(DDEL*DPSIDN)+ABS(DPSI*DDELDN)
       DET2=ABS(DDEL*DPSIDT)+ABS(DPSI*DDELDT)
       DET1=DET1+ABS(DPHI)*ABS(DDELDO*DPSIDN-DPSIDO*DDELDN)
       DET2=DET2+ABS(DPHI)*ABS(DDELDO*DPSIDT-DPSIDO*DDELDT)
       DET1=DET1+ABS(DNSR)*ABS(DDEDNR*DPSIDN-DPSDNR*DDELDN)
       DET2=DET2+ABS(DNSR)*ABS(DDEDNR*DPSIDT-DPSDNR*DDELDT)
       DET1=DET1+ABS(DNSI)*ABS(DDEDNI*DPSIDN-DPSDNI*DDELDN)
       DET2=DET2+ABS(DNSI)*ABS(DDEDNI*DPSIDT-DPSDNI*DDELDT)
       DET1=DET1/K1
       DET2=DET2/K1
C
C        DEFINE UNCERTAINTY DATA ARRAY
C            X(I) ANGLE OF INCIDENCE
       X(I)=PHI*RD
       YT(I)=DET1*100./T
       YN(I)=DET2
C         YT(I) % THICKNESS UNCERTAINTY  YN(I) FILM INDEX UNCERTAINTY
       GOTO 5000
C
C      ----------------------------------------------------------------
C            BEGIN CALC OF UNCERTAINTIES FOR BARE SUBSTRATE MODEL
C               CALCULATE DNSR AND DNSI AS DERIVED IN EQUATIONS
C                       (13) THROUGH (18)
C
1300   ZA=(NS*NS*(1.+SEC(PHI)*SEC(PHI))+NO*NO*(1.-SEC(PHI)*SEC(PHI)))
     1 /NS/TAN(PHI)
C
       ZD=2.*(RHO-1.)*NO*NO*SIN(PHI)*SIN(PHI)*TAN(PHI)*TAN(PHI)/
     1 NS/(1.+RHO)/(1.+RHO)/(1.+RHO)
C
       ZB=ZD*RHO*(0,1.)
```

```
C
       ZC=ZD*SEC(PSI)*SEC(PSI)*CEXP((0,1.)*DEL)
C
       DNSR=ABS(REAL(ZA)*DPHI)+ABS(REAL(ZB)*DDEL)
     1 +ABS(REAL(ZC)*DPSI)
C
       DNSI=ABS(AIMAG(ZA)*DPHI)+ABS(AIMAG(ZB)*DDEL)
     1 +ABS(AIMAG(ZC)*DPSI)
C
C           PUT RESULTS IN ANGLE OF INCIDENCE DATA ARRAY
C
       X(I)=PHI*RD
       YT(I)=DNSR
       YN(I)=DNSI
C
C      -------------------------------------------------------------
5000   CONTINUE
C
C                    DISPLAY RESULTS NEXT
C
C       THIS PROGRAM CONTAINS A PRINTOUT OF RESULTS COMMENTED OUT
C       AND INCLUDES VAX-11 RGL GRAPHICS TO PLOT UNCERTAINTIES AS A
C       FUNCTION OF ANGLE OF INCIDENCE.
C         THE GRAPHICS CAN ONLY BE USED WHEN COMPILED PROGRAM IS
C         LINKED WITH RGL GRAPHICS SUBROUTINES
C
C                   INITIALIZE GRAPHICS,CLEAR SCREEN AND TEXT,DRAW GRAPH
       CALL INITGR(5)
       CALL CLRSCR
       CALL CLRTXT
       CALL SCOLOR('GRAY3',1)
       CALL DPAPER('LIN',9,10,'LOG',3,9,'GRAY3')
C
C                   HEADINGS FOR PRINTOUT RESULTS OF FILM-SUBSTRATE MODEL
       IF (II .EQ. 1) GOTO 5250
C       WRITE(6,5200)
C       WRITE(4,5200)
C       FORMAT(/1X,'ANGLE OF INCIDENCE (deg)',3X,'PERCENT THICKNESS UNCER
C     1TAINTY',3X,'INDEX UNCERTAINTY'/)
C
C                   LABEL GRAPHS FOR FILM-SUBSTRATE MODEL
       CALL LNAXIS('XB','ANGLE OF INCIDENCE (deg)',0,
     190.,.TRUE.)
       CALL SCOLOR('GRAY1',2)
       CALL LNAXIS('YL','THICKNESS ERROR DT/T (%)',.1,100.,
     1.TRUE.)
       CALL SCOLOR('GRAY2',3)
       CALL LNAXIS('YR','INDEX ERROR DNF',.001,1.,.TRUE.)
       GOTO 5300
5250   CONTINUE
C                   HEADING FOR PRINTOUT RESULTS OF BARE SUBSTRATE MODEL
C       WRITE(6,5260)
```

```
C       WRITE(4,5260)
C       FORMAT(/1X,'ANGLE OF INCIDENCE (deg)',2X,'INDEX(REAL) UNCERTAIN
C     1TY',2X,'INDEX(IMAGINARY) UNCERTAINTY'/)
C
C                    LABEL GRAPHS FOR BARE SUBSTRATE MODEL
       CALL LNAXIS('XB','ANGLE OF INCIDENCE (deg)',0,
     190.,.TRUE.)
       CALL SCOLOR('GRAY1',2)
       CALL LNAXIS('YL','SUBSTRATE INDEX ERROR DNSR',.001,1.,
     1.TRUE.)
       CALL SCOLOR('GRAY2',3)
       CALL LNAXIS('YR','SUBSTRATE INDEX ERROR DNSI',.001,1.,
     1.TRUE.)
C
C                    LIST DATA
5300   CONTINUE
C       DO 6000 J=1,89
C       WRITE(4,5400) X(J),YT(J),YN(J)
C       WRITE(6,5400) X(J),YT(J),YN(J)
C       FORMAT(5X,F10.3,20X,F12.5,20X,F9.5)
C       CONTINUE
C
C                      GRAPH DATA
       CALL PDATA(89,X,YT,'L','GRAY1',,1,.FALSE.,,)
       CALL PDATA(89,X,YN,'R','GRAY2',,9,.FALSE.,,)
C
       CALL SCOLOR('GRAY3',1)
C
C           END OF MAIN PROGRAM
       END
```

FEDERAL INFORMATION PROCESSING STANDARD SOFTWARE SUMMARY

01. Summary date Yr. Mo. Day: 8 5 0 8 0 1

02. Summary prepared by (*Name and Phone*): Deane Chandler-Horowitz (301) 921-3625

03. Summary action: New ☒ Replacement ☐ Deletion ☐

Previous Internal Software ID

04. Software date Yr. Mo. Day: 8 5 0 6 1 0

05. Software title: Semiconductor Measurement Technology: A FORTRAN Program for analysis of the uncertainty in the ellipsometric determination of the thickness and refractive index of a film on a substrate or the refractive index of a bare substrate

06. Short title: ERROR.FOR

07. Internal Software ID

08. Software type
☐ Automated Data System
☒ Computer Program
☐ Subroutine/Module

09. Processing mode
☒ Interactive
☐ Batch
☐ Combination

10. Application area

General
☐ Computer Systems Support/Utility
☒ Scientific/Engineering
☐ Bibliographic/Textual
☐ Management/Business
☐ Process Control
☐ Other

Specific
Analysis of ellipsometric accuracy

11. Submitting organization and address

Semiconductor Electronics Division
National Bureau of Standards
Gaithersburg, MD 20899

12. Technical contact(s) and phone

Deane Chandler-Horowitz
(301) 921-3625

13. Narrative

The program performs the following functions: user can choose either the bare substrate or film substrate model; user inputs ellipsometric data (wavelength of light, angle of incidence, etc.); computes from the known input uncertainties the ellipsometric output uncertainty in either the film's thickness and refractive index or the substrate's refractive index; a graph of uncertainty as a function of angle of incidence is plotted.

14. Keywords

ellipsometry; bare-substrate model; film-substrate model; thickness uncertainty; refractive index uncertainty

15. Computer manuf'r and model DEC VAX 11/780	16. Computer operating system VMS 4.0	17. Programing language(s) FORTRAN	18. Number of source program statements 766
19. Computer memory requirements 55 KB	20. Tape drives one for program loading	21. Disk/Drum units none	22. Terminals 1 video VT 125

23. Other operational requirements

24. Software availability: Available ☒ Limited ☐ In-house only ☐

25. Documentation availability: Available ☒ Inadequate ☐ In-house only ☐

A user's manual is available as NBS Special Publication 400-78.

26. FOR SUBMITTING ORGANIZATION USE

NBS-114A (REV. 2-80)

U.S. DEPT. OF COMM. **BIBLIOGRAPHIC DATA SHEET** *(See instructions)*	1. PUBLICATION OR REPORT NO. NBS/SP-400/78	2. Performing Organ. Report No.	3. Publication Date May 1986

4. TITLE AND SUBTITLE

Semiconductor Measurement Technology: Analytic Analysis of Ellipsometric Errors

5. AUTHOR(S)

Deane Chandler-Horowitz

6. PERFORMING ORGANIZATION *(If joint or other than NBS, see instructions)*

National Bureau of Standards
Department of Commerce
Gaithersburg, MD 20899

7. Contract/Grant No.

8. Type of Report & Period Covered

Final

9. SPONSORING ORGANIZATION NAME AND COMPLETE ADDRESS *(Street, City, State, ZIP)*

Same as item 6

10. SUPPLEMENTARY NOTES

Library of Congrss Catalog Card Number: 86-600541

☐ Document describes a computer program; SF-185, FIPS Software Summary, is attached.

11. ABSTRACT *(A 200-word or less factual summary of most significant information. If document includes a significant bibliography or literature survey, mention it here)*

A computer program is given that contains an explicit ellipsometric error analysis. The program can identify the ellipsometric inaccuracies for any ellipsometer, can be used to determine which parameters contribute the most to the overall measurement inaccuracy, and can lead one to an optimum measurement procedure. A FORTRAN program that performs the evaluation of the partial derivative expressions needed to analyze ellipsometric measurement uncertainties is listed. The program determines the uncertainty in the calculation of the refractive index of a bare isotropic substrate or the uncertainty in the determination of the thickness and refractive index of a nonabsorbing film on a substrate of known refractive index. These are the two most commonly used surface models used in ellipsometry performed at single angle of incidence and a single wavelength. The program input parameters include the wavelength of the light, the angle of incidence and its uncertainty, and the uncertainties in the ellipsometric parameters Δ and ψ. They also include in the ambient-substrate model an estimated value for the substrate's refractive index, and in the film-substrate model the refractive index of the substrate and its uncertainty and estimated values for the film's refractive index and thickness. The case of the conventional null ellipsometer utilizing a quarter-wave plate is treated to find the uncertainties in Δ and ψ from the uncertainties in the polarizer and analyzer null values and the waveplate constants.

12. KEY WORDS *(Six to twelve entries; alphabetical order; capitalize only proper names; and separate key words by semicolons)*

bare substrate model; ellipsometry; film substrate model; FORTRAN program; measurement uncertainties; systematic errors.

13. AVAILABILITY

☒ Unlimited
☐ For Official Distribution. Do Not Release to NTIS
☒ Order From Superintendent of Documents, U.S. Government Printing Office, Washington, D.C. 20402.
☐ Order From National Technical Information Service (NTIS), Springfield, VA. 22161

14. NO. OF PRINTED PAGES

36

15. Price

☆ U.S. GOVERNMENT PRINTING OFFICE: 1986 - 491-070 - 265/40091

USCOMM-DC 6043-P80

NBS Technical Publications

Periodical

Journal of Research—The Journal of Research of the National Bureau of Standards reports NBS research and development in those disciplines of the physical and engineering sciences in which the Bureau is active. These include physics, chemistry, engineering, mathematics, and computer sciences. Papers cover a broad range of subjects, with major emphasis on measurement methodology and the basic technology underlying standardization. Also included from time to time are survey articles on topics closely related to the Bureau's technical and scientific programs. Issued six times a year.

Nonperiodicals

Monographs—Major contributions to the technical literature on various subjects related to the Bureau's scientific and technical activities.

Handbooks—Recommended codes of engineering and industrial practice (including safety codes) developed in cooperation with interested industries, professional organizations, and regulatory bodies.

Special Publications—Include proceedings of conferences sponsored by NBS, NBS annual reports, and other special publications appropriate to this grouping such as wall charts, pocket cards, and bibliographies.

Applied Mathematics Series—Mathematical tables, manuals, and studies of special interest to physicists, engineers, chemists, biologists, mathematicians, computer programmers, and others engaged in scientific and technical work.

National Standard Reference Data Series—Provides quantitative data on the physical and chemical properties of materials, compiled from the world's literature and critically evaluated. Developed under a worldwide program coordinated by NBS under the authority of the National Standard Data Act (Public Law 90-396). NOTE: The Journal of Physical and Chemical Reference Data (JPCRD) is published quarterly for NBS by the American Chemical Society (ACS) and the American Institute of Physics (AIP). Subscriptions, reprints, and supplements are available from ACS, 1155 Sixteenth St., NW, Washington, DC 20056.

Building Science Series—Disseminates technical information developed at the Bureau on building materials, components, systems, and whole structures. The series presents research results, test methods, and performance criteria related to the structural and environmental functions and the durability and safety characteristics of building elements and systems.

Technical Notes—Studies or reports which are complete in themselves but restrictive in their treatment of a subject. Analogous to monographs but not so comprehensive in scope or definitive in treatment of the subject area. Often serve as a vehicle for final reports of work performed at NBS under the sponsorship of other government agencies.

Voluntary Product Standards—Developed under procedures published by the Department of Commerce in Part 10, Title 15, of the Code of Federal Regulations. The standards establish nationally recognized requirements for products, and provide all concerned interests with a basis for common understanding of the characteristics of the products. NBS administers this program as a supplement to the activities of the private sector standardizing organizations.

Consumer Information Series—Practical information, based on NBS research and experience, covering areas of interest to the consumer. Easily understandable language and illustrations provide useful background knowledge for shopping in today's technological marketplace.

Order the **above** *NBS publications from: Superintendent of Documents, Government Printing Office, Washington, DC 20402.*

Order the **following** *NBS publications—FIPS and NBSIR's—from the National Technical Information Service, Springfield, VA 22161.*

Federal Information Processing Standards Publications (FIPS PUB)—Publications in this series collectively constitute the Federal Information Processing Standards Register. The Register serves as the official source of information in the Federal Government regarding standards issued by NBS pursuant to the Federal Property and Administrative Services Act of 1949 as amended, Public Law 89-306 (79 Stat. 1127), and as implemented by Executive Order 11717 (38 FR 12315, dated May 11, 1973) and Part 6 of Title 15 CFR (Code of Federal Regulations).

NBS Interagency Reports (NBSIR)—A special series of interim or final reports on work performed by NBS for outside sponsors (both government and non-government). In general, initial distribution is handled by the sponsor; public distribution is by the National Technical Information Service, Springfield, VA 22161, in paper copy or microfiche form.

U.S. Department of Commerce
National Bureau of Standards
Gaithersburg, MD 20899

Official Business
Penalty for Private Use $300